

Spectral Approximation for Quasiperiodic Jacobi Operators

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Abstract. Quasiperiodic Jacobi operators arise as mathematical models of quasicrystals and in more general studies of structures exhibiting aperiodic order. The spectra of these self-adjoint operators can be quite exotic, such as Cantor sets, and their fine properties yield insight into the associated quantum dynamics, that is, the one-parameter unitary group that solves the time-dependent Schrödinger equation. Quasiperiodic operators can be approximated by periodic ones, the spectra of which can be computed via two finite dimensional eigenvalue problems. Since long periods are necessary for detailed approximations, both computational efficiency and numerical accuracy become a concern. We describe a simple method for numerically computing the spectrum of a period- K Jacobi operator in $O(K^2)$ operations, then use the algorithm to investigate the spectra of Schrödinger operators with Fibonacci, period doubling, and Thue–Morse potentials.

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1. Introduction

For given sets of parameters $\{a_n\}, \{b_n\} \in \ell^\infty(\mathbb{Z})$, the corresponding *Jacobi operator* $\mathcal{J} : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$ is defined entrywise by

$$(\mathcal{J}\psi)_n = a_{n-1}\psi_{n-1} + b_n\psi_n + a_n\psi_{n+1} \quad (1.1)$$

for all $\{\psi_n\} \in \ell^2(\mathbb{Z})$. When there exists a positive integer K such that

$$a_n = a_{n+K}, \quad b_n = b_{n+K} \quad \text{for all } n \in \mathbb{Z},$$

the Jacobi operator is said to be *periodic* with *period* K . Here we are interested in computing the spectrum $\sigma(\mathcal{J})$ of such an operator when the period K is very long, as a route to high fidelity numerical approximations of the

more intricate spectra of operators with aperiodic coefficients. These spectra are important, as they can help us understand the quantum dynamics of solutions to the time-dependent Schrödinger equation [31].

The spectrum of a period- K Jacobi operator can be calculated from classical Floquet–Bloch theory, the relevant highlights of which we briefly recapitulate for later reference. (Our presentation most closely follows Toda [48, Ch. 4]; see also, e.g., [44, Ch. 5], [46, Ch. 7], [49].) For a scalar E , any solution to $\mathcal{J}\psi = E\psi$ satisfies

$$\begin{bmatrix} \psi_{pK+1} \\ \psi_{pK} \end{bmatrix} = M_K^p \begin{bmatrix} \psi_1 \\ \psi_0 \end{bmatrix} \quad (1.2)$$

for each $p \in \mathbb{Z}$, where $M_K \equiv M_K(E)$ denotes the 2×2 *monodromy matrix*

$$M_K = \begin{bmatrix} \frac{E-b_K}{a_K} & -\frac{a_{K-1}}{a_K} \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} \frac{E-b_2}{a_2} & -\frac{a_1}{a_2} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{E-b_1}{a_1} & -\frac{a_K}{a_1} \\ 1 & 0 \end{bmatrix}. \quad (1.3)$$

Note that

$$\det(M_K) = \frac{a_{K-1}}{a_K} \cdots \frac{a_1}{a_2} \frac{a_K}{a_1} = 1. \quad (1.4)$$

Now when \mathcal{J} is periodic, $E \in \sigma(\mathcal{J})$ provided $\mathcal{J}\psi = E\psi$ with bounded nontrivial $\psi = \{\psi_n\}$,¹ which by (1.2) and (1.4) requires the eigenvalues of M_K to have unit modulus. From

$$\det(\gamma - M_K) = \gamma^2 - \operatorname{tr}(M_K)\gamma + 1, \quad (1.5)$$

where $\operatorname{tr}(\cdot)$ denotes the trace, the eigenvalues of M_K have unit modulus when

$$-2 \leq \operatorname{tr}(M_K) \leq 2. \quad (1.6)$$

Since $\operatorname{tr}(M_k)$ is a degree- K polynomial in E , in principle we can find $\sigma(\mathcal{J})$ by solving the two polynomial equations $\operatorname{tr}(M_K(E)) = \pm 2$, giving $\sigma(\mathcal{J})$ as the union of K real intervals. For large K such numerical computations can incur significant errors, as illustrated in [14, Sec. 7.1]. Alternatively, note that if $[\psi_1, \psi_0]^T$ is an eigenvector of M_K associated with eigenvalue $\gamma = e^{i\theta}$, then by definition (1.1) and periodicity, $\mathcal{J}\psi = E\psi$ and $\psi_{K+j} = \gamma\psi_j$ imply

$$\begin{bmatrix} b_1 & a_1 & & & e^{-i\theta}a_K \\ a_1 & b_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & b_{K-1} & a_{K-1} \\ e^{i\theta}a_K & & & a_{K-1} & b_K \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{K-1} \\ \psi_K \end{bmatrix} = E \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{K-1} \\ \psi_K \end{bmatrix},$$

where all unspecified entries in the matrix equal zero. Solving this $K \times K$ symmetric matrix eigenvalue problem for any $\theta \in [0, 2\pi)$ gives K points in $\sigma(\mathcal{J})$, one in each of the K intervals. We can compute $\sigma(\mathcal{J})$ directly by noting

¹The spectrum of a Jacobi operator \mathcal{J} is given by the closure of the set of $E \in \mathbb{R}$ for which a nontrivial polynomially bounded solution to $\mathcal{J}\psi = E\psi$ exists. When \mathcal{J} is periodic, one either has a bounded solution or all solutions grow exponentially on at least one half-line.

that $\theta = 0$ and $\theta = \pi$ give the endpoints of these intervals. We shall thus focus on the two $K \times K$ symmetric matrices

$$\mathbf{J}_{\pm} = \begin{bmatrix} b_1 & a_1 & & & \pm a_K \\ a_1 & b_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & b_{K-1} & a_{K-1} \\ \pm a_K & & & a_{K-1} & b_K \end{bmatrix}. \quad (1.7)$$

More precisely, enumerating the $2K$ eigenvalues of \mathbf{J}_+ and \mathbf{J}_- such that

$$E_1 < E_2 \leq E_3 < E_4 \leq \cdots \leq E_{2K-1} < E_{2K} \quad (1.8)$$

(strict inequalities separate eigenvalues from \mathbf{J}_+ and \mathbf{J}_-), then

$$\sigma(\mathcal{J}) = \bigcup_{j=1}^K [E_{2j-1}, E_{2j}]. \quad (1.9)$$

This discussion suggests three ways to compute the spectrum (1.9):

1. For a fixed E , test if $E \in \sigma(\mathcal{J})$ by explicitly calculating $\text{tr}(M_k(E))$ and checking if (1.6) holds;
2. Construct the degree- K polynomial $\text{tr}(M_K(E))$ and find the roots of $\text{tr}(M_K(E)) = \pm 2$;
3. Compute the eigenvalues of the two $K \times K$ symmetric matrices \mathbf{J}_{\pm} .

The first method gives a fast way to test if $E \in \sigma(\mathcal{J})$ for a given E , but is an ineffective way to compute the entire spectrum. The second method suffers from the numerical instabilities mentioned earlier. The third approach is most favorable, but $O(K^3)$ complexity and numerical inaccuracies in the computed eigenvalues become a concern for large K .

Jacobi operators with long periods arise as approximations to Schrödinger operators with aperiodic potentials. For one special case (the almost Mathieu potential), Thouless [47] and Lamoureux [29] proposed an $O(K^2)$ algorithm to compute the spectra of \mathbf{J}_{\pm} for the period- K approximation. Section 2 describes a simpler $O(K^2)$ algorithm that does not exploit special properties of the potential, and so applies to any period- K Jacobi operator. Section 3 addresses aperiodic potentials in some detail, showing how their spectra can be covered by those of periodic approximations. Section 4 shows application of our algorithm to estimate the fractal dimension of the spectrum for aperiodic operators with potential given by primitive substitution rules.

2. Algorithm

The conventional algorithm for finding all eigenvalues of a general symmetric matrix \mathbf{A} first requires the application of unitary similarity transformations to reduce the matrix to tridiagonal form (in which all entries other than those on the main diagonal and the first super- and sub-diagonals are zero). This transformation is the most costly part of the eigenvalue computation: for a

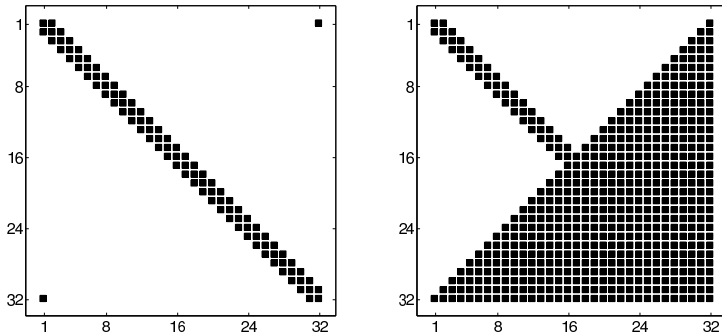


FIGURE 1. The nonzero pattern of \mathbf{J}_{\pm} for $K = 32$ (left) and an illustration of all the entries that are nonzero at some point in the transformation of \mathbf{J}_{\pm} to tridiagonal form using the conventional plane rotation approach (right).

$K \times K$ matrix, the reduction takes $O(K^3)$ operations, while the eigenvalues of the tridiagonal matrix can be found to high precision in $O(K^2)$ further operations [38, §8.15]. When many entries of \mathbf{A} are zero, one might exploit this structure to perform fewer elementary similarity transformations. This is the case when \mathbf{A} is banded: $a_{j,k} = 0$ when $|j - k| > b$, where b is the *bandwidth* of \mathbf{A} . For fixed b , the tridiagonal reduction takes $O(K^2)$ operations as $K \rightarrow \infty$.

The matrix \mathbf{J}_{\pm} in (1.7) is tridiagonal plus entries in the $(1, K)$ and $(K, 1)$ positions that give it bandwidth $b = K$. One might still hope to somehow exploit the zero structure to quickly reduce \mathbf{J}_{\pm} to tridiagonal form. Unfortunately, the transformation that eliminates the $(1, K)$ and $(K, 1)$ entries creates new nonzero entries where once there were zeros, starting a cascade of new nonzeros whose sequential elimination leads again to $O(K^3)$ complexity. Figure 1 shows how the conventional approach to tridiagonalizing a sparse matrix (using Givens plane rotations) eventually creates $O(K^2)$ nonzero entries, requiring $O(K^2)$ storage and $O(K^3)$ floating point operations.

The challenge is magnified by the eigenvalues themselves. As described in Section 3, we approximate aperiodic operators whose spectra are Cantor sets, implying that the eigenvalues of $\sigma(\mathbf{J}_{\pm})$ will be tightly clustered. The accuracy of these computed eigenvalues is critical to the applications we envision (e.g., estimating the fractal dimension of the Cantor sets), warranting use of extended (quadruple) precision arithmetic that magnifies the cost of $O(K^3)$ operations. Moreover, these studies often examine a family of operators over many parameter values (e.g., as the $\{b_n\}$ terms are scaled), so expedient algorithms are helpful even when K is tractable for a single matrix.

Thouless [47] and, in later, more complete work, Lamoureux [29] provide an explicit unitary matrix \mathbf{Q}_{\pm} such that $\mathbf{Q}_{\pm}^* \mathbf{J}_{\pm} \mathbf{Q}_{\pm}$ is tridiagonal in the special case of the almost Mathieu potential,

$$a_n = 1, \quad b_n = 2\lambda \cos(2\pi(n\alpha + \theta)),$$

where α is a rational approximation to an irrational parameter of true interest, and λ and θ are constants. This transformation gives an $O(K^2)$ algorithm for computing $\sigma(\mathbf{J}_\pm)$, but relies on the special structure of the potential.

Alternatively, we note that one can compute all eigenvalues of \mathbf{J}_\pm in $O(K^2)$ time by simply reordering the rows and columns of \mathbf{J}_\pm to yield a matrix with small bandwidth that is independent of K . Recall that the nonzero pattern of a symmetric matrix \mathbf{A} can be represented as an undirected graph having vertices labeled $1, \dots, K$, with distinct vertices j and k joined by an edge if $a_{j,k} = a_{k,j} \neq 0$. (We suppress the loops corresponding to $a_{j,j} \neq 0$.) The graph for \mathbf{J}_\pm has a single cycle, shown in Figure 2 for $K = 8$. In the conventional labeling, the corner entries in the $(1, K)$ and $(K, 1)$ positions give an edge between vertices 1 and K . To obtain a matrix with narrow bandwidth, simply relabel the vertices in a breadth-first fashion starting from vertex 1, as illustrated in Figure 2. Now each vertex only connects to vertices whose labels differ by at most *two*: if we permute the rows and columns of the matrix in accord with the relabeling, the resulting matrix will have bandwidth 2 (i.e., a *pentadiagonal* matrix). More explicitly, define

$$p(j) = \begin{cases} 2j - 1, & j \in \{1, \dots, \lceil K/2 \rceil\}; \\ 2(K - j - 1), & j \in \{\lceil K/2 \rceil + 1, \dots, K\}. \end{cases}$$

Let $\mathbf{P} = [\mathbf{e}_{p(1)}, \mathbf{e}_{p(2)}, \dots, \mathbf{e}_{p(K)}]$, where \mathbf{e}_j is the j th column of the $K \times K$ identity matrix; then $\mathbf{P}\mathbf{J}_\pm\mathbf{P}^*$ has bandwidth $b = 2$. When $K = 8$,

$$\mathbf{J}_\pm = \begin{bmatrix} b_1 & a_1 & & & & & & \pm a_8 \\ a_1 & b_2 & a_2 & & & & & \\ & a_2 & b_3 & a_3 & & & & \\ & & a_3 & b_4 & a_4 & & & \\ & & & a_4 & b_5 & a_5 & & \\ & & & & a_5 & b_6 & a_6 & \\ & & & & & a_6 & b_7 & a_7 \\ \pm a_8 & & & & & & a_7 & b_8 \end{bmatrix}$$

is reordered to

$$\mathbf{P}\mathbf{J}_\pm\mathbf{P}^* = \begin{bmatrix} b_1 & \pm a_8 & a_1 & & & & & \\ \pm a_8 & b_8 & & a_7 & & & & \\ a_1 & & b_2 & a_2 & & & & \\ & a_7 & & b_7 & a_6 & & & \\ & & a_2 & b_3 & a_3 & & & \\ & & & a_6 & b_6 & a_5 & & \\ & & & & a_3 & b_4 & a_4 & \\ & & & & & a_5 & a_4 & b_5 \end{bmatrix},$$

where unspecified entries are zero. The tridiagonal reduction of banded symmetric matrices has been carefully studied, starting with Rutishauser² [42]; see [10] for contemporary algorithmic considerations. Such matrices can be

²Rutishauser was motivated by pentadiagonal matrices that arise in the addition of continued fractions.

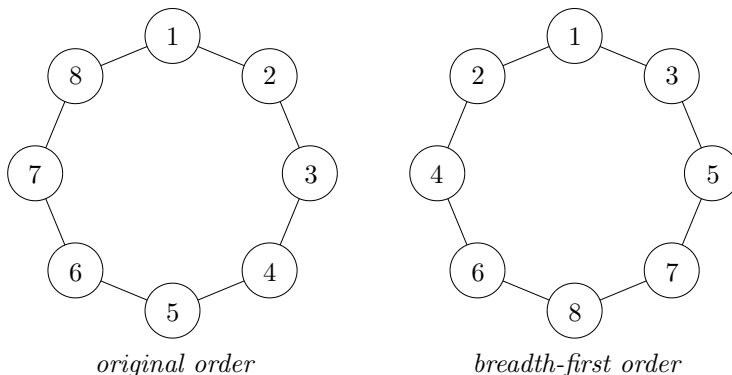
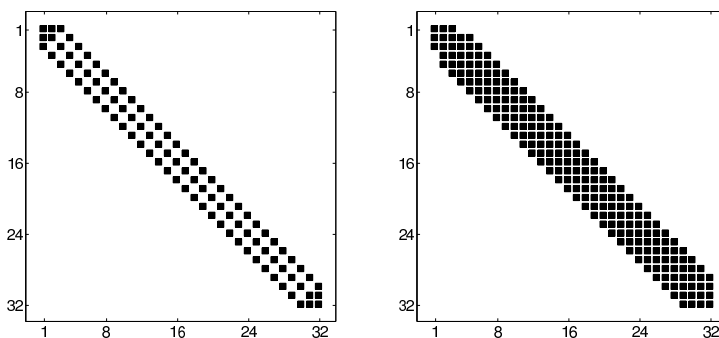
FIGURE 2. The vertex reordering scheme for $K = 8$.

FIGURE 3. Analogue of Figure 1 for the pentadiagonal matrix from the breadth-first ordering (left) and the nonzeros that arise in reduction of this matrix to tridiagonal form using the bulge-chasing approach (right).

reduced to tridiagonal form using Givens plane rotations applied in a “bulge-chasing” procedure that increases the bandwidth by one; Figure 3 shows the nonzero entries introduced by this reduction.³ Removing the $(j + 2, j)$ entry introduces a new entry in the third subdiagonal (a “bulge”) that is “chased” toward the bottom right with $O(K)$ additional Givens rotations, each of which requires $O(1)$ floating point operations. Performing this exercise for $j = 1, \dots, K - 2$ amounts to $O(K^2)$ work and $O(K)$ storage to reduce $\mathbf{P}\mathbf{J}_{\pm}\mathbf{P}^*$ to tridiagonal form, an improvement over the usual $O(K^3)$ work and $O(K^2)$ storage. (Our application does not require the eigenvectors of \mathbf{J}_{\pm} , so we do not store the transformations that tridiagonalize \mathbf{J}_{\pm} .)

One can compute a banded tridiagonalization using the LAPACK software library’s `dsbtrd` routine, or compute the eigenvalues directly with the

³An alternative method that finds the eigenvalues of a banded symmetric matrix directly in its band form is described in [38, §8.16]. This method, based on small Householder reflectors, is particularly effective when a small subset of the spectrum is sought.

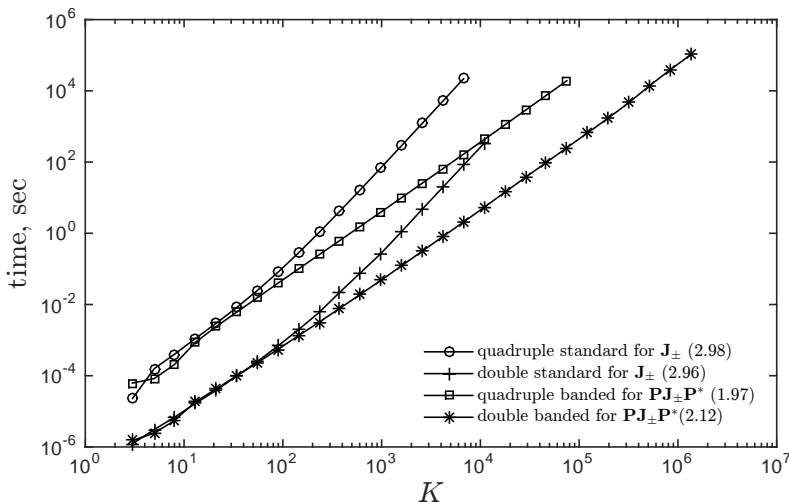


FIGURE 4. Performance of LAPACK's standard (`dsyev`) and banded (`dsbev`) symmetric eigensolvers in double and quadruple precision, applied to the Fibonacci model.

banded eigensolver `dsbev` [2]. (If $\mathbf{PJ}_{\pm}\mathbf{P}^*$ stored in sparse format, MATLAB's `eig` command will identify the band form and find the eigenvalues in $O(K^2)$ time.) We have benchmarked our computations in LAPACK with standard double precision arithmetic and a variant compiled for quadruple precision.⁴ When $a_n = 1$ and $b_n = 0$ for all n , the eigenvalues of \mathbf{J}_{\pm} are known in closed form [23]. With the reordering scheme described above, LAPACK returns the correct eigenvalues, up to the order of machine precision (roughly 10^{-16} for double precision and 10^{-34} for quadruple precision). Figure 4 compares the timing of the reordered scheme to the traditional dense matrix approach. In both double and quadruple precision, the $O(K^2)$ performance of the reordered approach offers a significant advantage. (These timings were performed on a desktop with a 3.30 GHz Intel Xeon E31245 processor, applied to the Fibonacci model described in the next section. The numbers in the legend indicate the slope of a linear fit of the last five data points, and each algorithm is averaged over the four Fibonacci parameters $\lambda = 1, 2, 3, 4$.)

3. Spectral theory for quasiperiodic Schrödinger operators

We focus on Jacobi operators that are *discrete Schrödinger operators*, that is, those operators for which the off-diagonal terms satisfy $a_n = 1$ for all n , and the *potential* $\{b_n\}$ varies in a deterministic but non-periodic fashion.⁵

⁴<http://icl.cs.utk.edu/lapack-forum/viewtopic.php?f=2&t=2739> gives compilation instructions.

⁵In *off-diagonal* models, $b_n = 0$ for all n , while the a_n coefficients vary aperiodically, see, e.g., [33, 50].

For several prominent examples the spectrum is a Cantor set; in other cases even a gross description of the spectral type has been elusive.

Periodic approximations lead to elegant covers of the spectra of the quasiperiodic operators,⁶ and while the arguments that produce these covers are now standard, there is not such a direct venue in the literature where this framework is quickly summarized. Consequently, we recapitulate the essential arguments for the reader unfamiliar with this landscape; those seeking greater detail can consult the more extensive survey [13]. In Section 4 we shall apply our algorithm to numerically compute the spectral covers described here.

A variety of quasiperiodic potentials have been investigated in the mathematical physics literature; for a survey, see, e.g., [18]. Most prominent is the *almost Mathieu operator* [25, 47], with potential

$$b_n = 2\lambda \cos(2\pi(n\alpha + \theta)) \quad (3.1)$$

for irrational α , nonzero *coupling constant* λ , and *phase* $\theta \in \mathbb{R}$. The spectrum of the almost Mathieu operator is a Cantor set for all irrational α , every θ , and every $\lambda \neq 0$ [3]. Moreover, the Lebesgue measure of the spectrum is precisely $4|1 - |\lambda||$ whenever α is irrational [4, Theorem 1.5]. Of particular interest is the Hausdorff dimension of the spectrum in the critical case $\lambda = 1$, about which very little is known; see [30] for some partial results.

Sturmian potentials take the form

$$b_n = \lambda \chi_{[1-\alpha, 1)}((n\alpha + \theta) \bmod 1), \quad (3.2)$$

where χ_S is the indicator function on the set $S \subset \mathbb{R}$ and α , λ , and θ play the same role as in (3.1). For such potentials the spectrum is a Cantor set of zero Lebesgue measure for all irrational α , nonzero λ and phases θ [8]. It is conjectured that for a fixed nonzero coupling λ , the Hausdorff dimension of the spectrum is constant on a set of α 's of full Lebesgue measure; currently, this is only known for $\lambda \geq 24$ [16, Theorem 1.2].

3.1. Quasiperiodic operators from substitution rules

Alternatively, aperiodic potentials can be constructed from primitive substitution rules. Unlike the almost Mathieu and Sturmian cases, the spectral type of the operators is not well-understood. Having spectrum of zero Lebesgue measure precludes the presence of absolutely continuous spectrum, a result known well before Damanik and Lenz proved zero-measure spectrum; see the main result of [28]. So far, numerous partial results exclude eigenvalues for particular substitution operators [8, 11, 12, 17, 26], and no results yet establish the existence of eigenvalues for any (two-sided) substitution operator. The construction is slightly more involved than previous examples, but since seeking a better understanding of substitution potentials is a motivation of this work, we describe these objects in detail.

⁶Except for the Almost Mathieu operator, the potentials we describe are not quasiperiodic in the classical sense of being almost periodic sequences with finitely generated frequency modules. However, the terminology is completely standard at this point.

Let $\mathcal{A} \subset \mathbb{R}$ be a finite set, called the *alphabet*.⁷ A *substitution* on \mathcal{A} is a rule that replaces elements of \mathcal{A} by finite-length words over \mathcal{A} . For example, the *period doubling* substitution, S_{PD} , is defined by the rules $\mathbf{a} \mapsto \mathbf{ab}$ and $\mathbf{b} \mapsto \mathbf{aa}$ over the two-letter alphabet $\mathcal{A} = \{\mathbf{a}, \mathbf{b}\}$ [9]. The *Thue–Morse* substitution uses the rules $\mathbf{a} \mapsto \mathbf{ab}$ and $\mathbf{b} \mapsto \mathbf{ba}$ [7, 20]. The *Fibonacci* potential [27, 36] can be viewed as a Sturmian potential with $\alpha = (\sqrt{5} - 1)/2$ and $\theta = 0$, or as a primitive substitution potential with rules $\mathbf{a} \mapsto \mathbf{ab}$, $\mathbf{b} \mapsto \mathbf{a}$. (The equivalence of these definitions follows from [8, Lemma 1b].) One can also study substitutive sequences on larger alphabets; for example, the *Rudin–Shapiro* substitution is defined on the four-symbol alphabet $\mathcal{A} = \{\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}\}$ by the rules $\mathbf{a} \mapsto \mathbf{ab}$, $\mathbf{b} \mapsto \mathbf{ac}$, $\mathbf{c} \mapsto \mathbf{db}$, and $\mathbf{d} \mapsto \mathbf{dc}$ [41, 43].

Each of the aforementioned examples enjoys a property known as *primitivity*, which can be described informally as the existence of an iterate which maps each letter to a word containing the full alphabet. More precisely, we say that a substitution S is *primitive* if there exists some $k \in \mathbb{Z}_+$ so that for every $\mathbf{a}, \mathbf{b} \in \mathcal{A}$, \mathbf{b} is a subword of $S^k(\mathbf{a})$.

We now describe how a primitive substitution rule leads to a quasiperiodic Schrödinger operator, focusing on period doubling as a concrete example. To obtain an aperiodic sequence, start with the symbol \mathbf{a} and form the sequence $w_k = S_{\text{PD}}^k(\mathbf{a})$ by iteratively applying the period doubling substitution rules, $\mathbf{a} \mapsto \mathbf{ab}$ and $\mathbf{b} \mapsto \mathbf{aa}$. The result is a sequence of finite words: $w_0 = \mathbf{a}$, $w_1 = \mathbf{ab}$, $w_2 = \mathbf{abaa}$, $w_3 = \mathbf{abaaabab}$, and so on. Notice that w_k is always a prefix of w_{k+1} . In particular, there is a well-defined limiting sequence,

$$x_{\text{PD}} = \lim_{k \rightarrow \infty} S_{\text{PD}}^k(\mathbf{a}) = \mathbf{abaaabababaaabaa} \dots, \quad (3.3)$$

with the property that x_{PD} is fixed by the period doubling substitution; sequences with this property are called *substitution words* for the substitution.

From a substitution word x_{PD} one can construct a quasiperiodic potential for a discrete Schrödinger operator. Given a coupling constant λ , take

$$\mathbf{a} = \lambda; \quad \mathbf{b} = 0; \quad b_n = n\text{th symbol of } x_{\text{PD}}. \quad (3.4)$$

One subtlety remains: the substitution word x_{PD} is a one-sided sequence, while our potentials are two-sided, i.e., we should specify b_n for all $n \in \mathbb{Z}$. To generate two-sided potentials, one considers an accumulation point of left-shifts of x_{PD} ; equivalently, one considers a two-sided sequence with the same local factor structure as x_{PD} . The details of this construction follow.

Suppose S is a primitive substitution on the finite alphabet $\mathcal{A} \subset \mathbb{R}$ and $x \in \mathcal{A}^{\mathbb{N}}$ is some substitution word thereof, i.e., $S(x) = x$. The *subshift* generated by S is the set of all two-sided sequences with the same local factor structure as x . More precisely,

$$\Omega_S = \{\omega \in \mathcal{A}^{\mathbb{Z}} : \omega_n \cdots \omega_m \text{ is a subword of } x \text{ for every } n \leq m\}. \quad (3.5)$$

Using primitivity of S , one can check that this definition of Ω_S does not depend upon the choice of substitution word. One can also generate the set

⁷We do not necessarily have to restrict our attention to alphabets consisting of real numbers, but this makes the definition of our subshift potentials in (3.7) somewhat simpler.

Ω_S via the following dynamical procedure. First, endow the sequence space $\mathcal{A}^{\mathbb{Z}}$ with some metric that induces the product topology thereupon, e.g.,

$$d(\omega, \omega') = \sum_{n \in \mathbb{Z}} \frac{1 - \delta_{\omega_n, \omega'_n}}{2^{|n|+1}}, \quad (3.6)$$

where $\delta_{a,b}$ denotes the usual Kronecker delta symbol. The sequences ω and ω' are close with respect to the metric in (3.6) if and only if they agree on a large window centered at the origin, so this metric does indeed induce the topology of pointwise convergence on Ω_S . One can check that Ω_S defined by (3.5) coincides precisely with the set of limits of convergent subsequences of the sequence $(T^n x)_{n=1}^{\infty}$, where T denotes the usual left shift $(T\omega)_n = \omega_{n+1}$. (There is a minor technicality here: since x is a one-sided sequence $(T^n x)_k$ is only well-defined for $n > |k|$ when k is negative.)

Primitivity of S implies that the topological dynamical system (Ω_S, T) is strictly ergodic [39, Proposition 5.2 and Theorem 5.6]. For each $\omega \in \Omega_S$, one obtains a Schrödinger operator H_ω on $\ell^2(\mathbb{Z})$ defined via

$$(H_\omega \psi)_n = \psi_{n-1} + \omega_n \psi_n + \psi_{n+1} \quad (3.7)$$

for each $n \in \mathbb{Z}$. (The right hand side of (3.7) makes sense, since we chose $\mathcal{A} \subseteq \mathbb{R}$.) Minimality of (Ω_S, T) implies ω -invariance of the spectrum.

Proposition 3.1. *Given Ω_S and H_ω as above, there is a uniform compact set Σ with the property that $\sigma(H_\omega) = \Sigma$ for every $\omega \in \Omega_S$.*

Proof. Given $\omega, \omega' \in \Omega_S$, there is a sequence $\{n_k\} \subset \mathbb{Z}$ with the property that $T^{n_k} \omega \rightarrow \omega'$ as $k \rightarrow \infty$. (This is a consequence of minimality of (Ω_S, T) , which follows from [39, Proposition 4.7], for example.) In particular,

$$H_{\omega'} = \text{s-lim}_{k \rightarrow \infty} H_{T^{n_k} \omega}.$$

By a standard strong approximation argument (e.g., [40, Theorem VIII.24]),

$$\sigma(H_{\omega'}) \subseteq \overline{\bigcap_{\ell=1}^{\infty} \bigcup_{k=\ell}^{\infty} \sigma(H_{T^{n_k} \omega})} = \sigma(H_\omega). \quad (3.8)$$

By symmetry, we can run the previous argument with the roles of ω and ω' reversed, so $\sigma(H_\omega) = \sigma(H_{\omega'})$. \square

This is the upshot of the previous proposition: if we want to study the spectrum of a two-sided substitutive Schrödinger operator *as a set*, then we can work with any member of the associated subshift.

One can avoid the construction needed to generate two-sided potentials by considering instead *half-line* Jacobi operators, $\mathcal{J}_+ : \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$. These operators are defined entrywise by (1.1) for $n \in \mathbb{N}$ with the normalization $\psi_0 = 0$ to make $(\mathcal{J}_+ \psi)_1$ well defined. If \mathcal{J}_+ denotes the Jacobi operator defined by $a_n \equiv 1$ and (3.4), and \mathcal{J} denotes a two-sided Jacobi operator generated in one of the two fashions just described, then by [44, Theorem 7.2.1],

$$\sigma_{\text{ess}}(\mathcal{J}_+) = \sigma(\mathcal{J}), \quad (3.9)$$

where $\sigma_{\text{ess}}(\cdot)$ denotes the essential spectrum. In particular, $\sigma(\mathcal{J}_+)$ and $\sigma(\mathcal{J})$ have the same Hausdorff dimension, since (3.9) implies that they coincide up to a countable set of isolated points.

3.2. Periodic approximations

All the classes of quasiperiodic models we have described have natural periodic approximations. For the almost Mathieu and Sturmian cases: replace the irrational α with a rational approximant; for the substitution rules: pick a starting symbol, generate a string from finitely many applications of the substitution rules, and repeat that string periodically. We seek high fidelity numerical approximations to these periodic spectra, as a vehicle for understanding properties of quasiperiodic models, such as the fractal dimension of the spectrum.

In the case of substitution rules, we shall describe how periodic approximations lead to an *upper bound* on the spectrum of the quasiperiodic operator. Again we focus on the period doubling substitution. Fix $S_{\text{PD}}, x_{\text{PD}}$ as before, choose some $\omega \in \Omega_{\text{PD}}$, and put $w_k^a = S^k(a)$ and $w_k^b = S^k(b)$. We generate periodic Schrödinger operators H_k^a and H_k^b by repeating the strings w_k^a and w_k^b periodically, giving H_k^a and H_k^b with coefficients having period 2^k . Moreover, we choose H_k^a and H_k^b in such a way that

$$H_\omega = \text{s-lim}_{k \rightarrow \infty} H_k^a = \text{s-lim}_{k \rightarrow \infty} H_k^b.$$

Define $\Sigma_k^a \equiv \sigma(H_k^a)$ and $\Sigma_k^b \equiv \sigma(H_k^b)$ for all $k \geq 0$. Application of strong approximation, as before, implies

$$\Sigma \subseteq \bigcap_{n=1}^{\infty} \overline{\bigcup_{k=n}^{\infty} \Sigma_k^a}, \quad \Sigma \subseteq \bigcap_{n=1}^{\infty} \overline{\bigcup_{k=n}^{\infty} \Sigma_k^b}. \quad (3.10)$$

These unions are too large to be computationally tractable, but the hierarchical structure of the periodic approximations saves the day. In these cases the monodromy matrices (1.3) take the forms

$$\begin{aligned} M_k^a(E) &= \begin{bmatrix} E - w_k^a(2^k) & -1 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} E - w_k^a(1) & -1 \\ 1 & 0 \end{bmatrix} \\ M_k^b(E) &= \begin{bmatrix} E - w_k^b(2^k) & -1 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} E - w_k^b(1) & -1 \\ 1 & 0 \end{bmatrix}, \end{aligned}$$

where now the subscript k denotes the k th iteration of the substitution rule, and hence a full period of length $K = 2^k$. Recalling the discriminant condition (1.6), define

$$x_k(E) \equiv \text{tr}(M_k^a(E)), \quad y_k(E) \equiv \text{tr}(M_k^b(E)).$$

As in (1.6), these functions encode the spectra of the periodic approximants, in that $\Sigma_k^a = \{E : |x_k(E)| \leq 2\}$ and $\Sigma_k^b = \{E : |y_k(E)| \leq 2\}$. The rules of the

period doubling substitution imply

$$M_{k+1}^a = M_k^b M_k^a \quad (3.11)$$

$$M_{k+1}^b = M_k^a M_k^a. \quad (3.12)$$

Applying the Cayley–Hamilton theorem ($M_k^2 - \text{tr}(M_k)M_k + I = 0$) to (3.11) and (3.12) yields

$$x_{k+1} = x_k y_k - 2 \quad (3.13)$$

$$y_{k+1} = x_k^2 - 2, \quad (3.14)$$

given in [9, eq. (1.9)]. Now (3.13) and (3.14) imply $\Sigma_{k+1}^a \cup \Sigma_{k+1}^b \subseteq \Sigma_k^a \cup \Sigma_k^b$ for all $k \geq 0$, thus reducing (3.10) to the more tractable

$$[\text{Period Doubling}] \quad \Sigma \subseteq \bigcap_{k=1}^{\infty} \Sigma_k^a \cup \Sigma_k^b. \quad (3.15)$$

The spectrum for the Thue–Morse substitution can be expressed in the same way, except that substitution rule replaces (3.13)–(3.14) with

$$x_{k+1} = x_{k-1}^2 (x_k - 2) + 2 \quad (3.16)$$

$$y_{k+1} = x_{k+1}. \quad (3.17)$$

Reasoning as in the period doubling case, (3.16)–(3.17) implies

$$[\text{Thue–Morse}] \quad \Sigma \subseteq \bigcap_{k=1}^{\infty} \Sigma_k^a \cup \Sigma_{k+1}^a. \quad (3.18)$$

Notice that (3.15) and (3.18) are not identical. In general, the covers of the spectrum obtained via this approach depend quite strongly on the chosen substitution. Note, however, that the same formula (3.18) holds for the Fibonacci substitution. The recursive relationships in (3.13)–(3.14) and (3.16)–(3.17) are known as the *trace maps* for the period doubling and Thue–Morse potentials. Similar trace maps can be constructed for arbitrary substitutions; see [5, Theorem 1] and [6, Theorem 1] for their description.

Figure 5 depicts the covers $\Sigma_k^a \cup \Sigma_k^b$ for the period doubling potential and $\Sigma_k^a \cup \Sigma_{k+1}^a$ for Thue–Morse as λ increases from zero with $k = 7$, giving an impression of how rapidly the covering intervals shrink as λ increases. Notice the quite different nature of the spectra obtained from these two substitution rules. Similar figures for the Fibonacci spectrum are shown in [14]. (The algorithm described in the last section enables such computations for much larger values of k , but the resulting figures become increasingly difficult to render due to the number and narrow width of the covering intervals.)

4. Numerical calculation of periodic covers

In this section, we apply the algorithm described in Section 2 to compute the spectral covers for quasiperiodic operators from substitution rules described in Section 3. We begin with some calculations that emphasize the need for

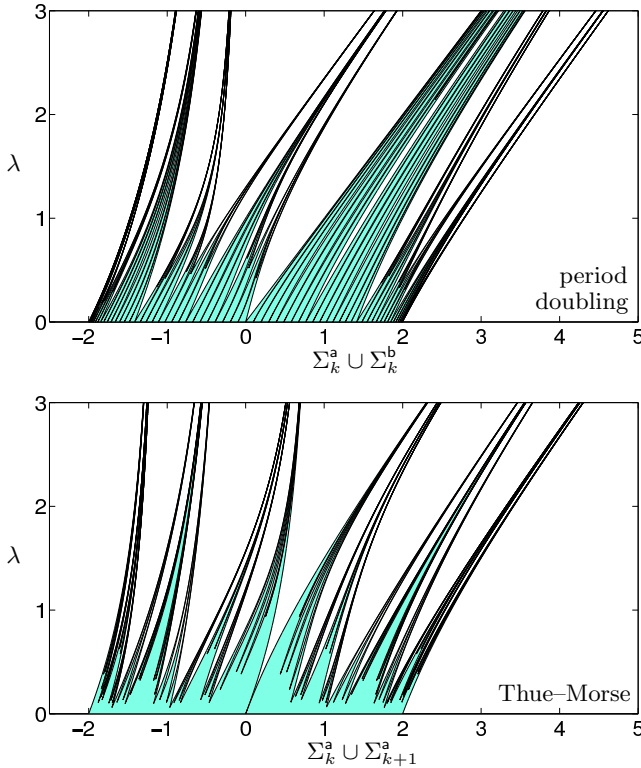


FIGURE 5. Spectral covers for the period doubling ($\Sigma_k^a \cup \Sigma_k^b$) and Thue–Morse ($\Sigma_k^a \cup \Sigma_{k+1}^a$) potentials as a function of the coupling constant λ , for $k = 7$.

higher precision arithmetic to resolve the spectrum, then estimate various spectral quantities for these quasiperiodic operators.

4.1. Necessity for extended precision

High fidelity spectral approximations for quasiperiodic Schrödinger operators are tricky to compute due not only to the complexity of the eigenvalue problem, but also considerations of numerical precision. The LAPACK symmetric eigenvalue algorithms are expected to compute eigenvalues of the $K \times K$ matrix \mathbf{J}_\pm accurate to within $p(K)\|\mathbf{J}_\pm\|\varepsilon_{\text{mach}}$ [2, p. 104], where $p(K)$ is a “modestly growing function of K ” and $\varepsilon_{\text{mach}}$ denotes the machine epsilon value for the floating point arithmetic system (on the order of 10^{-16} for double precision and 10^{-34} for quadruple precision [1]). Figure 6 shows the width of the smallest interval in the approximation Σ_k^a for the period doubling and Thue–Morse potentials, as computed in double and quadruple precision arithmetic for various values of λ . As λ increases, this smallest interval shrinks ever quicker. Comparing double and quadruple precision values, one sees that for even moderate values of $K = 2^k$, double precision is unable to accurately

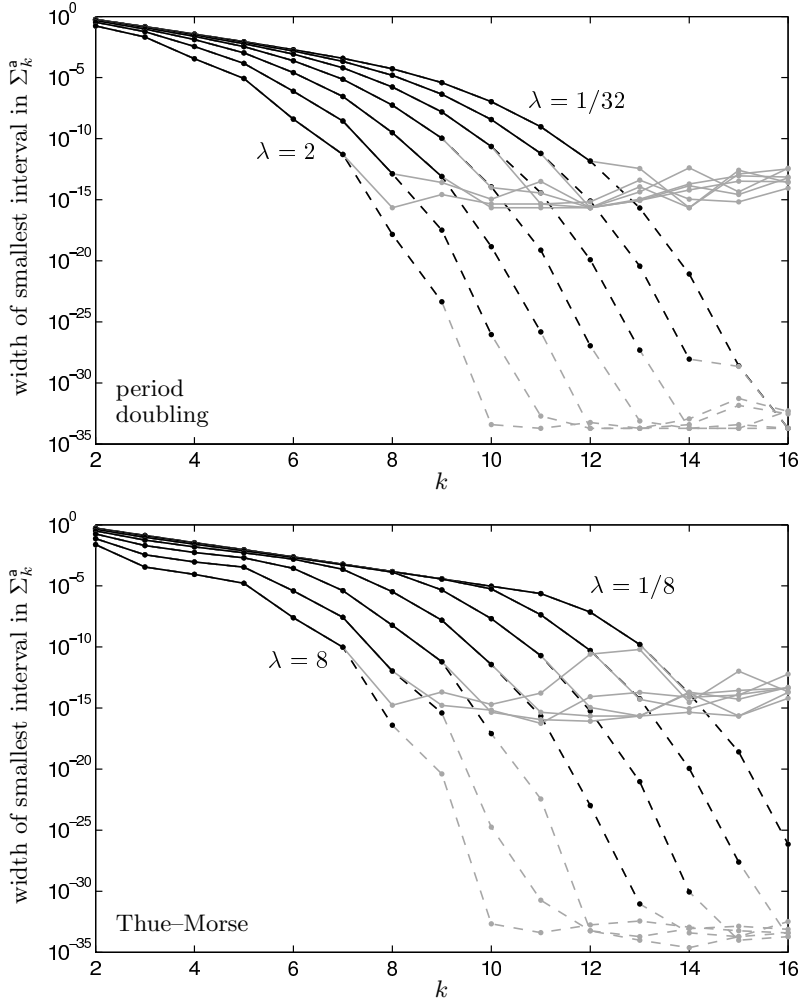


FIGURE 6. Minimum interval length in Σ_k^a for a range of λ values (powers of two) for the period doubling and Thue–Morse potentials. The solid line shows double precision, the dashed line quadruple precision. Black data points are believed to be correct to plotting accuracy; gray ones are not.

resolve the spectrum.⁸ (Similar numerical errors will be observed for the original matrix \mathbf{J}_\pm . Since it only permutes matrix entries, our algorithm does not introduce any new instabilities.)

⁸The calculations of fractal dimension and gaps that follow were performed in quadruple precision arithmetic, and we generally restricted the values of λ and k to obtain numerically reliable results. In the event the numerical results violate the ordering of eigenvalues of \mathbf{J}_+ and \mathbf{J}_- in (1.8), any offending interval is replaced by one of width $20\varepsilon_{\text{mach}}$ centered at the midpoint of the computed eigenvalues.

4.2. Approximating fractal dimensions

The quasiperiodic spectrum Σ is known to be a Cantor set for the Fibonacci, period doubling, and Thue–Morse potentials for all $\lambda > 0$, suggesting calculation of the fractal dimensions of these sets as functions of λ . We begin with two standard definitions; see, e.g., [22, 37].

Definition 4.1. Given $A \subset \mathbb{R}$ and some $\alpha \in [0, 1]$, let

$$h^\alpha(A) \equiv \lim_{\Delta \rightarrow 0} \inf_{\Delta\text{-covers}} \sum_{m \geq 1} |B_m|^\alpha,$$

where a Δ -cover of A is defined to be collection $\{B_m\}_{m \geq 1}$ of intervals such that $A \subset \bigcup_{m \geq 1} B_m$ and $|B_m| < \Delta$ for each m . The *Hausdorff dimension* of A is then

$$\dim_H(A) \equiv \inf\{\alpha : h^\alpha(A) < \infty\}.$$

Definition 4.2. Given $A \subset \mathbb{R}$, let $N_A(\varepsilon)$ denote the number of intervals of the form $[j\varepsilon, (j+1)\varepsilon)$, $j \in \mathbb{Z}$, that have a nontrivial intersection with A . The upper and lower box counting dimensions of A are

$$\dim_B^\pm(A) \equiv \lim_{\varepsilon \rightarrow 0} \sup_{\inf} \frac{\log N_A(\varepsilon)}{\log 1/\varepsilon};$$

when these agree, the result is the *box-counting dimension* of A , $\dim_B(A)$.

The analysis in the last section provides natural covering sets for Σ , which we denote as C_k (i.e., for period doubling, $C_k \equiv \Sigma_k^a \cup \Sigma_k^b$; for Fibonacci and Thue–Morse, $C_k \equiv \Sigma_k^a \cup \Sigma_{k+1}^a$). We estimate $\dim_H(\Sigma)$ using a heuristic proposed by Halsey et al. [24]. Enumerate the n_k intervals in C_k as $\{B_{k,m}\}$:

$$C_k = \bigcup_{m=1}^{n_k} B_{k,m}.$$

Approximating the Hausdorff dimension

- 1: **Input:** two consecutive covers $C_{k,\lambda}, C_{k+1,\lambda}$ of the Cantor spectrum.
 - 2: Construct the function $f(\alpha) \equiv \sum_{m=1}^{n_k} |B_{k,m}|^\alpha - \sum_{m=1}^{n_{k+1}} |B_{k+1,m}|^\alpha$.
 - 3: Compute root α_k of $f(\alpha)$ in the interval $[0, 1]$.
 - 4: **Output:** α_k as the approximation to the dimension.
-

For the Fibonacci case, Damanik et al. [15] proved upper and lower bounds on $\dim_H(\Sigma)$ for $\lambda \geq 8$ in terms of the functions $S_u(\lambda) = 2\lambda + 22$ and $S_l(\lambda) = \frac{1}{2}(\lambda - 4 + \sqrt{(\lambda - 4)^2 - 12})$. To benchmark our method, we compare the approximate dimension with the upper and lower bounds, as shown in Figure 7, indeed obtaining satisfactory results. Figure 8 shows estimates to $\dim_H(\Sigma)$ drawn from spectral covers for $k = 6, \dots, 10$, with good convergence in k in the small λ regime. The narrow covering intervals for large λ and k pose a significant numerical challenge, even in quadruple precision arithmetic.

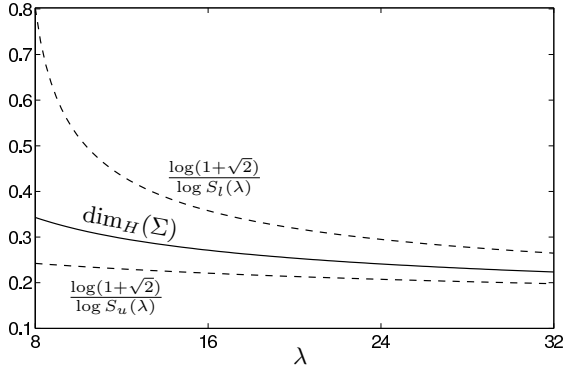


FIGURE 7. Estimates of $\dim_H(\Sigma)$ for the Fibonacci operator (solid line) computed from $\Sigma_k^a \cup \Sigma_{k+1}^a$ ($k = 15, 16$), obeying the upper and lower bounds from [15].

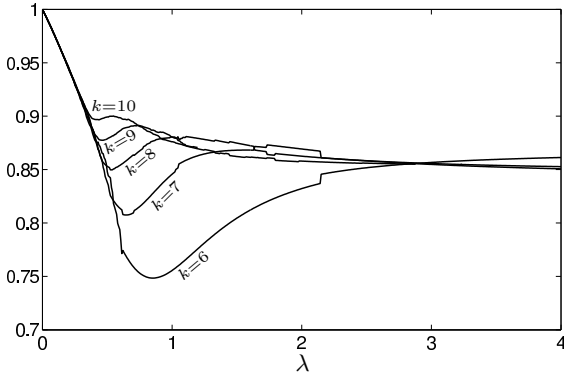


FIGURE 8. Estimates of $\dim_H(\Sigma)$ for the period-doubling operator using consecutive covers $\Sigma_k^a \cup \Sigma_k^b$ and $\Sigma_{k+1}^a \cup \Sigma_{k+1}^b$, for $k = 6, \dots, 10$. (The $k = 9$ and $k = 10$ plots do not show the full range of λ values, due to the numerical challenge of working with large k and λ .)

The bounds from [15] imply $\dim_H(\Sigma) \rightarrow 0$ like $\log(1 + \sqrt{2})/\log(\lambda)$ as $\lambda \rightarrow \infty$ for the Fibonacci case. In contrast, Liu and Qu [32] recently showed that for the Thue–Morse operator, $\dim_H(\Sigma)$ is bounded away from zero as $\lambda \rightarrow \infty$. Interestingly, the approximation scheme described above does not yield consistent results for Thue–Morse, perhaps a reflection of the exotic behavior identified in [32]. As an alternative, in Figure 9 we show estimates of the box-counting dimension for Thue–Morse. Since for any finite k the covers comprise the finite union of real intervals, $\log(N_{C_k}(\varepsilon))/\log(1/\varepsilon) \rightarrow 1$ as $\varepsilon \rightarrow 0$. However, for finite ε the shape of the curves in Figure 9 can suggest rough values for $\dim_B(\Sigma)$; cf. [45]. Figure 10 repeats the experiment for period doubling; note that the plot for $\lambda = 4$ shows good agreement with the estimate for $\dim_H(\Sigma)$ seen in Figure 8. (The Hausdorff and box counting

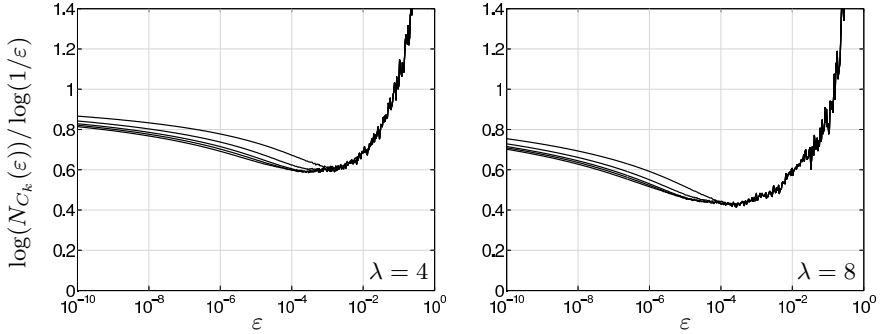


FIGURE 9. Estimates of $\dim_B(\Sigma)$ for the Thue–Morse operator for $\lambda = 4, 8$, using covers C_k with $k = 5, \dots, 9$.

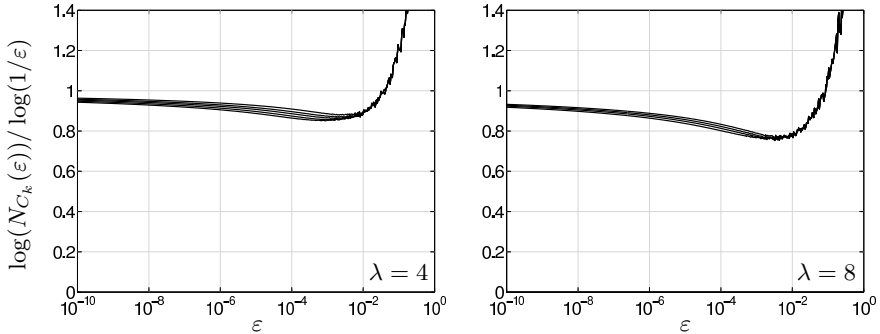


FIGURE 10. Estimates of $\dim_B(\Sigma)$ for the period-doubling operator for $\lambda = 4, 8$, using covers C_k with $k = 5, \dots, 9$.

dimensions need not be equal; considerable effort was devoted over the years to showing $\dim_H(\Sigma) = \dim_B(\Sigma)$ for all $\lambda > 0$ for the Fibonacci case, with the complete result obtained only recently [19].)

The spectral covers we have described can behave in rather subtle ways. To illustrate this fact, Figure 11 shows the largest gap in the Thue–Morse cover $\Sigma_k^a \cup \Sigma_{k+1}^a$ as a function of the parameter λ . Bellisard [7] showed that, for the aperiodic model, this gap should behave like $\lambda^{\log 4 / \log 3}$ as $\lambda \rightarrow 0$. The covers satisfy this characterization for intermediate values of λ , but appear to behave instead like λ^2 as $\lambda \rightarrow 0$. The larger the value of k (hence the longer the periodic approximations), the larger the range of λ values that are consistent with Bellisard’s spectral asymptotics. This scenario provides another justification for the study of large- k approximations: for this potential, one must consider large k to approximate the spectrum adequately for small λ .

Our algorithm also expedites study of the square Hamiltonians \mathcal{J}_{sq} acting on $\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$ via

$$(\mathcal{J}_{\text{sq}}\psi)_{m,n} = \psi_{m-1,n} + \psi_{m,n-1} + (b_m + b_n)\psi_{m,n} + \psi_{m+1,n} + \psi_{m,n+1}.$$

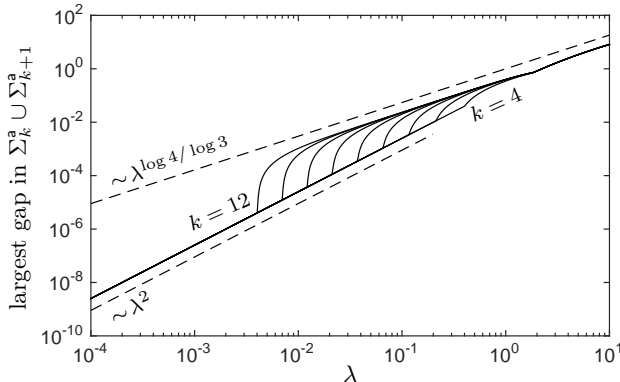


FIGURE 11. Computed values of the largest gap in the cover $\Sigma_k^a \cup \Sigma_{k+1}^a$ of the Thue–Morse spectrum, along with Bellisard’s asymptotic description $\lambda^{\log 4 / \log 3}$. As k increases, the covers obey the asymptotics for smaller values of λ .

The spectrum of this operator is $\Sigma + \Sigma$, where Σ is the spectrum of the standard 1-dimensional operator with potential $\{b_n\}$. When Σ is a Cantor set, $\Sigma + \Sigma$ could be an interval, a union of intervals, a *Cantorval*, or a Cantor set; see, e.g., [34, 35, 37]. For further details and examples for the Fibonacci case, see [14] and the computations, based on $\sigma(\mathbf{J}_\pm)$, of Even-Dar Mandel and Lifshitz [21]. For the period doubling and Thue–Morse potentials, Figure 12 illustrates how the covers of the spectra for these square Hamiltonians develop in λ , revealing values of λ for which $\Sigma + \Sigma$ cannot comprise a single interval.

5. Conclusion

We have presented a simple $O(K^2)$ algorithm to numerically compute the spectrum of a period- K Jacobi operator that can be implemented in a few lines of code, then we used this algorithm to estimate spectral quantities associated with quasiperiodic Schrödinger operators derived from substitution rules. The algorithm facilitates study of long-period approximations and extensive parameter studies across a family of operators. Yet even with the efficient algorithm, the accuracy of the numerically computed eigenvalues must be carefully monitored, or even enhanced with extended precision computations. This tool can expedite numerical experiments to help formulate conjectures about spectral properties for a range of quasiperiodic operators.

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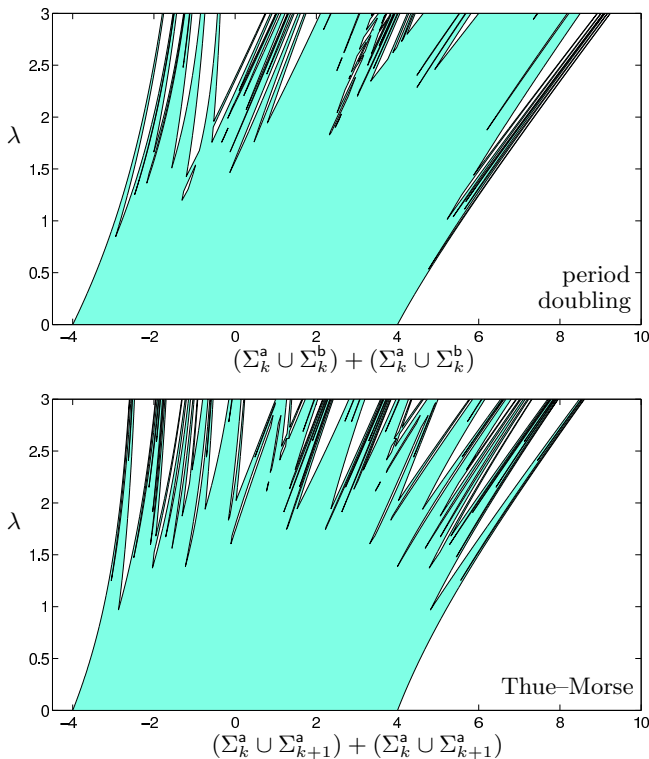


FIGURE 12. Spectral covers for the square Hamiltonian for period doubling and Thue–Morse substitutions, with $k = 4$.

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